The "Virtual Density" Principle of Neutronics and Its Application to Geometric Perturbation Theory

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INTRODUCTION

We desire to rapidly predict the reactivity and flux distribution effects due to geometric distortions in fast reactors. These include bowing, flowering, and core expansion. We employ conventional perturbation theory but find its direct application to these distortions to be inadequate for our purposes. Thus, we revive an old but little-known theory that we call the "virtual density" principle of neutronics. We demonstrate that it is universally applicable to established neutronics methods, verify that it is extremely expeditious for uniform core expansions, and state how it can also be applied to non-uniform geometric distortions.

THE "VIRTUAL DENSITY" PRINCIPLE OF NEUTRONICS

General Theory

For now, let us consider an idealized uniform core expansion in which every material in the entire reactor swells by the same factor. Of course, in real scenarios the liquid coolant would not swell along with other materials, but we will neglect that effect for now. Let the reactor volume be V, and let any given material atom density be N. If mass is conserved, then N will vary inversely proportional to V.

$$N \propto \frac{1}{V} \quad (1)$$

If we let λ be any given neutron mean free path in the core, then λ will vary proportional to V.

$$\lambda \propto \frac{1}{\Sigma_t} = \frac{1}{N\sigma_t} \propto V \quad (2)$$

Here we have shown what will actually occur physically in this idealized uniform core expansion scenario. During core expansion, the neutron mean free path increases at a rate greater than the rate at which all linear core dimensions increase. Thus, the net reactivity change will be negative - the negative reactivity effect due to reduced material densities will overcome the positive reactivity effect due to increased core size, and so the net effect will be increased leakage. This is true for

any arbitrary reactor except an infinite 1-D slab, for which the net reactivity change will be precisely zero.

However, what if we wished to keep reactivity constant during a uniform core expansion of an arbitrary reactor? We would need to scale up the neutron mean free path proportional to the core linear dimensions ($V^{1/3}$) - not proportional to core volume (V), which is what actually occurs physically.

$$\lambda \propto V^{1/3} \rightarrow N \propto V^{-1/3} \quad (3)$$

Thus, if we uniformly expand the core volume V and simultaneously reduce all core material densities proportional to $V^{1/3}$, the neutron leakage rate will not change. Of course, it follows that the relative magnitudes of neutron fluxes between internal core regions will not change such that the spatial neutron distribution will not change. Furthermore, because the relative proportions of all materials in the core will not change, the neutron energy spectrum will not change. Thus, the reactor is essentially "scaled up" without any change to reactivity or to spatial or spectral flux distributions.

A Theorem and its Corollary

Theorem: Swelling all linear dimensions of *any* given reactor by a certain factor while simultaneously reducing all material densities by that same factor will result in *exactly* zero change to reactivity and flux distributions.

Corollary: The reactivity and flux distribution effects of a uniform core expansion (or contraction) can be *exactly* replicated by manipulating material densities with no change to core geometry.

Past Work

Equating a uniform core expansion to a uniform core density change is not an entirely new concept. S. B. Shikov proposed what he called "similarity theory" in 1959 [1]. Since then, it has been applied to determine uniform thermal core expansion reactivity coefficients. The design of the BN-800, a sodium fast reactor currently under construction in Russia, employed some of these methods [2]. However, these "virtual density" methods (as we shall call them) have not been applied to non-uniform geometric distortions.

A "Virtual" Uniform Core Expansion

Now let us examine a more realistic scenario. Consider a sodium fast reactor (SFR). We will define a uniform radial core expansion as a uniform increase in pin pitch. Thus, the core expands uniformly in the radial direction but not at all in the axial direction. If the core swells from radius R_1 to a larger radius R_2, the homogenized fuel and structure densities in each assembly will decrease by a factor of $(R_2/R_1)^2$. However, the homogenized sodium density will increase by the factor $(R_1/R_2)^2[(R_2/R_1)^2 - f]/(1-f)$, where f is the volume fraction of fuel and structure. As the pin pitch increases, sodium flows into the core.

Given our theorem and corollary, we can exactly replicate the reactivity and flux distribution effects of such a uniform core expansion without expanding the core at all. Instead of enlarging the core, we simply contract the neutron mean free paths by increasing all material densities by a factor of R_2/R_1 above what they

k_{eff} = 1.04. The vacuum boundary condition provides plenty of leakage. The fuel and structure volume fraction is f = 0.62, although the square assemblies are homogenized with no pin-level detail.

We perform the diffusion simulation with a MATLAB finite difference code integrated with the PETSc and SLEPc linear algebra packages. We call this MaPS. It uses the SLEPc generalized eigenvalue solver with Arnoldi iterations. We utilize 33-group cross-sections produced by the code MC**2, which is tailored to process fast reactor cross-sections [3].

We perform the deterministic transport simulation with OpenMOC, an open-source method of characteristics (MOC) code developed at MIT in early 2012. We utilize the identical 33-group MC**2 cross-sections.

We perform the continuous-energy Monte Carlo simulation with MCNP5 [4]. We utilize cross-sections in the Evaluated Nuclear Data Format (ENDF/B-VII.0).

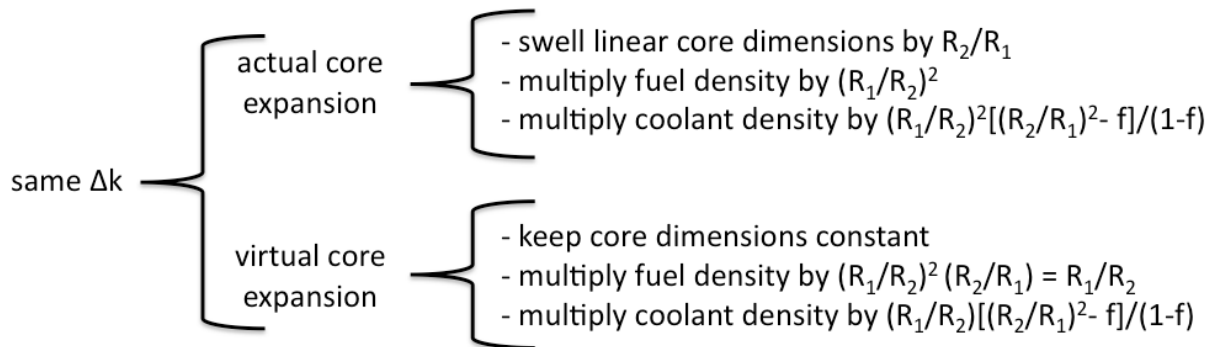In each of these simulations, we compare the reactivity change induced by an "actual" core expansion

Fig. 1. The processes of "actual" and "virtual" uniform radial core expansions.

would be during an "actual" core expansion. For example, we increase the fuel and structure densities by a factor of R_2/R_1 after they have already been decreased by a factor of $(R_2/R_1)^2$ during the "actual" expansion. Thus, the net effect of the "virtual" expansion is that the fuel and structure densities are decreased by a factor of R_2/R_1, which is less than the factor they would have been decreased by during an "actual" expansion. See Fig. 1 for a summary.

Equivalence in Diffusion, Deterministic Transport, and Monte Carlo

To demonstrate the universality of this "virtual density" principle, we will demonstrate that it is equally valid in diffusion, deterministic transport, and Monte Carlo simulations.

In all three simulations, we use the same very simple geometry – a 5x5 array of square enriched uranium assemblies surrounded by a square sodium blanket. Without expansion, this reactor is a bit supercritical with

to that induced by a "virtual" core expansion (as defined in Fig. 1), and we see that they are *precisely* equivalent. Tables I, II, and III show the complete results. Indeed, the "virtual density" principle is universal, and we could reproduce similar results for *any* core geometry.

Note that the MCNP results agree surprisingly well. In all four cases, the 1σ k_{eff} uncertainty is 1 pcm, and all four sets of two k_{eff} values round to the same nearest pcm. Although this is not the most likely outcome, it is certainly not unlikely enough to cause concern. We examine Shannon entropy to ensure that the fission source distribution has converged.

Table I. Diffusion k_{eff} Values for "Actual" and "Virtual" Uniform Core Expansions (10^{-10} convergence)

R_2/R_1	actual k_{eff}	virtual k_{eff}	k_{eff} error (pcm)
1	1.0335072167	N/A	N/A
1.001	1.0332285619	1.0332285619	0.00000
1.01	1.0307346898	1.0307346898	0.00000
1.1	1.0071396247	1.0071396247	0.00000
2	0.8708997837	0.8708997837	0.00000

Table II. MOC k_{eff} Values for "Actual" and "Virtual" Uniform Core Expansions (10^{-6} convergence)

R_2/R_1	actual k_{eff}	virtual k_{eff}	k_{eff} error (pcm)
1	1.041188	N/A	N/A
1.001	1.040907	1.040907	0.0
1.01	1.038388	1.038388	0.0
1.1	1.014440	1.014440	0.0
2	0.872294	0.872294	0.0

Table III. Monte Carlo k_{eff} Values for "Actual" and "Virtual" Uniform Core Expansions (4 billion histories)

R_2/R_1	actual k_{eff}	virtual k_{eff}	k_{eff} error (pcm)
1	1.03867±0.00001	N/A	N/A
1.001	1.03841±0.00001	1.03841±0.00001	0 ± 2
1.01	1.03593±0.00001	1.03593±0.00001	0 ± 2
1.1	1.01257±0.00001	1.01257±0.00001	0 ± 2
2	0.87772±0.00001	0.87772±0.00001	0 ± 2

APPLICATION TO PERTURBATION THEORY

Why does this "virtual density" principle matter? It's a neat trick, but directly computing a "virtual" core expansion is no less computationally intensive than directly computing an "actual" core expansion in diffusion theory. If we are simulating core expansions by solving the full-core diffusion eigenvalue problem, there is no advantage to the "virtual" core expansion.

However, if we wish to save time and effort by evaluating core expansion reactivity effects using perturbation theory, then the "virtual" expansion is tremendously expeditious. Material density perturbations are much more straightforward to evaluate than geometry perturbations (or boundary perturbations). Material density perturbations require nothing more than a simple, traditional (first or second order) perturbation theory calculation. This is identical in process to computing the reactivity density coefficient of a material.

In order to test this for a realistic scenario, we construct a Fast Flux Test Facility (FFTF) benchmark model in 2-D hexagonal geometry using MaPS [5].

We compare the reactivity effects due to directly computing an "actual" expansion with those predicted by applying first order perturbation theory to a "virtual" expansion. See Figs. 2 and 3, which show the first order reactivity shift prediction and its error, respectively. Essentially, one can predict the reactivity shift due to an x% radial core expansion to less than x%. All the diffusion meshes here are the same - only six triangular mesh cells per hexagonal assembly.

We should compare these results to those obtained by Knutson, et. al. in 1981 [6]. They attempted to predict the reactivity shift due to a 100 mil = 1/10 inch uniform radial expansion of FFTF. This very small shift corresponds to a radial increase of about 0.2%. They could use first order perturbation theory to predict their diffusion eigenvalue solution to no less than 12% error. They subsequently perform analysis to conclude that nearly all of this error arises from spatial effects rather than spectral effects. First order perturbation theory uses the unperturbed spatial and spectral flux distributions. Material density perturbations are simple, because they include only spectral error. Geometry perturbations, however, include both spectral error and (usually much larger) spatial error. However, because the "virtual density" method essentially converts geometric perturbations into density perturbations, it completely eliminates the spatial error, leaving only the (usually much smaller) spectral error. Thus, for the same 100 mil radial expansion of FFTF, we can achieve 0.13% error with first order perturbation theory. Evidently, these FFTF engineers of the 1980s were unaware of this "virtual density" principle already being applied in the Soviet Union.

CONCLUSIONS AND ONGOING WORK

We have shown that this "virtual density" principle of neutronics can convert many geometric perturbations into precisely equivalent material density perturbations. Essentially, this technique eliminates all spatial error in geometric perturbation theory, leaving only spectral error. In the case of uniform core expansions, this allows first order perturbation theory to predict the reactivity shift with an error that is orders of magnitude smaller than achievable with direct application of perturbation theory.

Furthermore, these "virtual density" techniques can greatly simplify many problems in boundary perturbation theory. Most notably, evaluating an arbitrary 1-D slab boundary perturbation becomes quite simple relative to current techniques [7]. We have begun to apply these methods to non-uniform core distortions, such as assembly-level bowing and flowering. If these methods can be applied to whole cores, they can also be applied to small regions within cores. Work is ongoing at MIT.

NOMENCLATURE

f = volume fraction of fuel and structure
N = atom density
R = core radius
V = volume
λ = neutron mean free path
Σ_t = macroscopic total cross-section
σ_t = microscopic total cross-section

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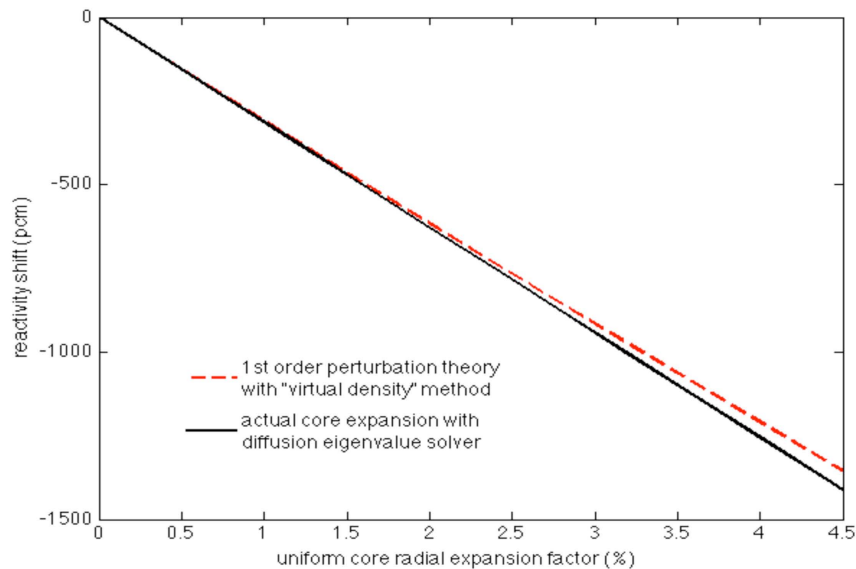
Fig. 2. Reactivity shift as a function of uniform core radial swelling for a 2-D FFTF benchmark.
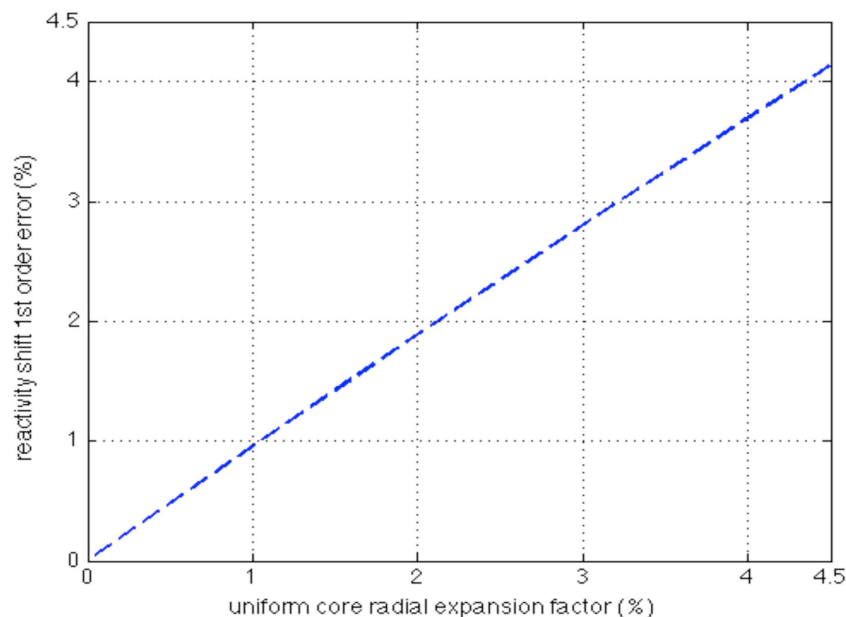

Fig. 3. First order error in reactivity shift due to uniform radial swelling of the 2-D FFTF benchmark. This is the error between the two curves shown in Fig. 2.